Some Thoughts on UQ Challenges for Multi-physics Applications

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ICIS Workshop on Verification/Uncertainty Quantification

Aug 7-13, 2011

This work was performed under the auspices of the U.S. Department of Energy by
Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344

What is uncertainty quantification? My current favorite definition

Uncertainty quantification involves the

- **identification (where the uncertainties are),**
  - **Physics model, data, environment, …**
- **characterization (what form they are),**
  - **Parametric (bounds, PDF, beliefs), model form**
- **propagation (how they evolve, forward/inverse),**
  - **Choice of method influenced by model characteristics**
- **analysis (what are the impacts, quantitative) , and**
  - **Sensitivity analysis, risk analysis, …**
- **reduction**

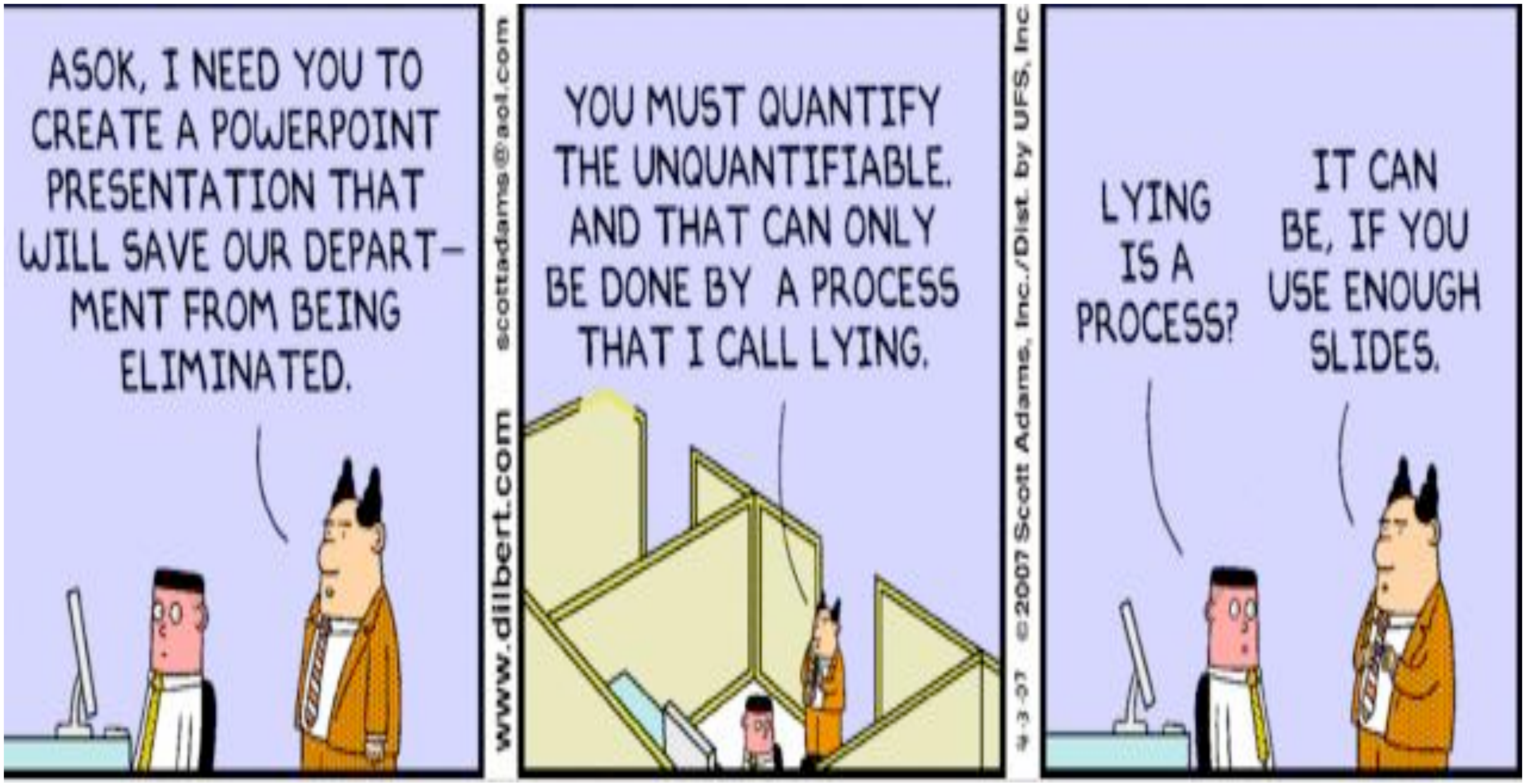
of uncertainties in simulation models.

Not including method development

In order to perform UQ on a given application, we need

- An UQ process
  - A well-thought plan with a well-defined objective
  - Consisting of a number of steps
  - Each step may require expert judgment or suitable UQ methods
- Relevant UQ methods (forward propagation, SA, calibration)
  - Intrusive methods
  - Non-intrusive methods
  - Hybrid (intrusive+nonintrusive) methods
- Adequate hardware/software infrastructure to perform UQ
  - Job management: scheduling, monitoring
  - Data processing
  - Analysis and visualization of results

Every UQ study should start with a plan (process)



For example, a UQ process may include the following steps, which identify key UQ methodologies needed

1. Define the objective of the UQ study (e.g. quantify risk)
2. Problem specification (model, assumptions, QOI, available data)
3. Perform verification experiments (to assess numerical errors)
4. Preliminary parameter identification and selection
5. Prescribe initial parameter distributions (literature, expert opinion)
6. Integrate observation data into models
7. Parameter screening
8. Build inexpensive surrogates/emulators
9. Uncertainty/Sensitivity analysis
10. Risk/predictability assessment
11. Expert reviews, documentation

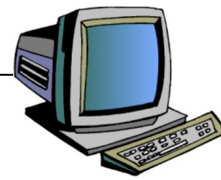
communication

Defining a UQ process early on will help to identify UQ methodologies needed for a given application.

Identification of the sources of uncertainty (so many!)

Mathematical model/simulation code

Design parameters



Model responses

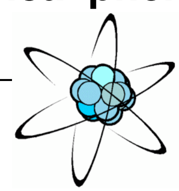
Uncertainties in:
- Design parameter values
- initial/boundary conditions
- Measurement errors
- surrounding environment

Uncertainties in:
- Physics sub-models
  * imprecise/simplified physics
  * data-driven empirical models
- Sub-model couplings
- Missing physics
- Model implementation
- Roundoff errors
- Algorithmic errors (e.g. MC)
- Discretization errors

- Measurement errors
- Data scarcity
- Noisy data

Physical phenomenon

Experiments



Observations

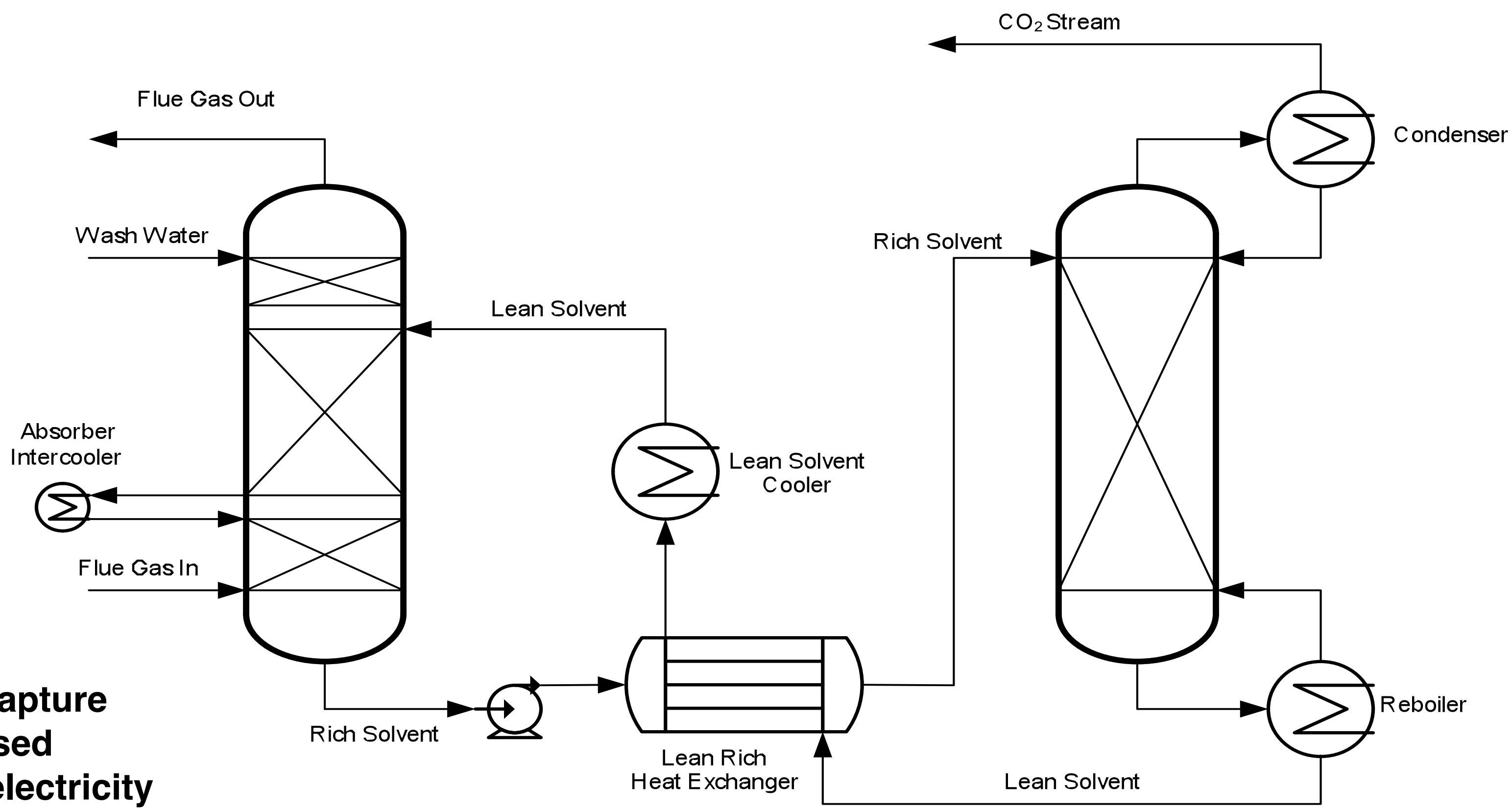
** need to identify ALL key sources of uncertainties????

All UQ analysis are wrong, but how wrong do they have to be not to be useful?

identification

A systematic methodology for identification??

An Example: Carbon Capture System



% CO2 capture
Steam used
Cost of electricity

Sources of uncertainties: (simplified models)
flue gas composition, chemical kinetics, mass transfers, geometries, corrosion, external conditions,
Chemical reaction model, modeling of the absorber column

identification

Nature of uncertainties in other applications

- Uncertainties in the use of approximate models
- Uncertainties in physics parameters/models
- Uncertainties in integral measurements and derived quantities
- Uncertainty in the uncertainties of the data
- Ambiguities in historical data
- Uncertainty effect of surrogate materials
  - In related small scale experiments
- Effect of material aging
- Experimental data less relevant with time
- Model used to predict scale-up (untested) systems

identification

A systematic methodology for identification??

Classification of uncertainties

- Known pdfs
- Unknown pdfs
  - use intervals or belief functions
  - missing physics (will give systematic errors)
- Mixed
  - known pdfs, unknown distribution parameters
- Model form uncertainties
  - many possible equations to represent the submodels
  - each sub-model may have its own mixed uncertainties
- Errors (considered as uncertainties?)
  - discretization errors, roundoff errors, algorithmic errors

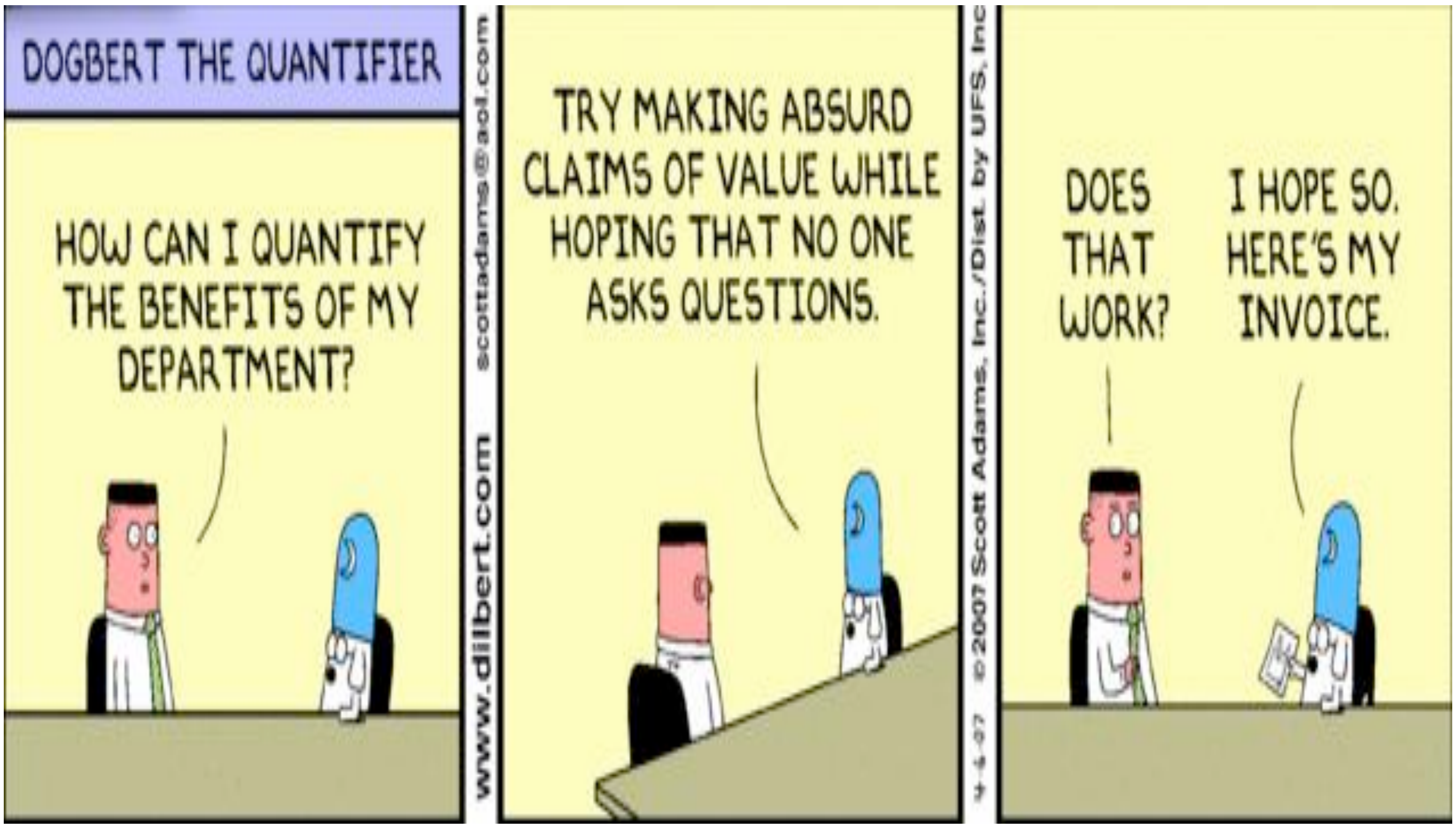
characterization

Uncertainty Characterization

- We always say: obtain parameter uncertainties from expert judgment, literature, and experimental data
- Most application scientists do not know for sure the parameter distributions
- Many papers that compare models against data do not include estimation of posterior distributions
- Most parameter distributions/bounds are based on calibration/validation results, but many data suffer the problem: difficult to characterize data uncertainties
  - Uncertainties of uncertainties
- How to prescribe uncertainties to handle extrapolation?
- Insufficient characterization may have significant effect on UQ analysis results.

characterization

The creditability of UQ results depends a lot on the characterization of uncertainties



characterization

Some UQ objectives

- Compute output distributions input uncertainties
- Identify parameters that contribute most to output uncertainties
  - Quantify such contributions
  - Research prioritization
- Characterize parameter distributions (feasible subspace) that best fit a collection of systems
- Study how uncertainties in data distributions affect output uncertainty
- Study parameter correlation induced by observation data
- Identify systematic errors (unknown unknowns?)
- Use calibrated parameters to predict hold-out systems (near-by)
- Parameter study (e.g. explore nonlinear and interaction effects)
- Analyze uncertainties due to alternative sub-model forms
- Evaluate risks (e.g. failure to meet regulations) in view of uncertainties
- Find optimal settings while taking uncertainties into consideration

Propagation

Multi-physics Model Characteristics Encountered

- Simplified/empirical physics sub-models abound
- Models are expensive to evaluate (hours on many processors)
- Nonlinear input-output relationships anticipated
- Abrupt changes/discontinuities possible but not encountered yet
- High-dimensionality of the uncertain parameters (10's -100's or more)
- Untypical correlation between uncertain parameters (from calibration)
- Mainly epistemic uncertainties (aleatoric forthcoming)
- Uncertainties in uncertainty bounds and distribution parameters
- Model form uncertainties abound (have not addressed them yet)
- Different observation data (component, subsystem, full system)
- Data scarcity and uncertainties about data uncertainties
- Model operating at different regime than experiments (extrapolation)
- Uncertainties mixed with numerical errors
- Unknown unknowns (unknown processes, unknown couplings)

Propagation

Implication of the model characteristics of multi-physics models on the selection of UQ methodologies/methods

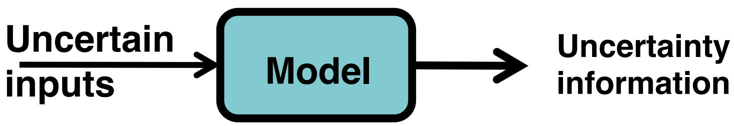
- Classical methods such as SRC may not be sufficient
- Local perturbation-based sensitivity analysis may not be sufficient
  - Global sensitivity analysis methods are needed
- Dimension reduction/variable selection methods may be needed
  - Nonparametric methods needed for nonlinear problems
- Many runs may be needed to resolve nonlinearities/interaction
  - Adaptive sampling may be needed if complexity is local
- Parametric surrogate methods may not be feasible
  - Non-parametric surrogates/response surfaces may be needed
- Hierarchical/multi-stage data fusion methods may be needed
  - Empty set (zero posteriors, systematic errors) may be encountered

Proper selection of methods are critical in defensible UQ analysis.

Propagation

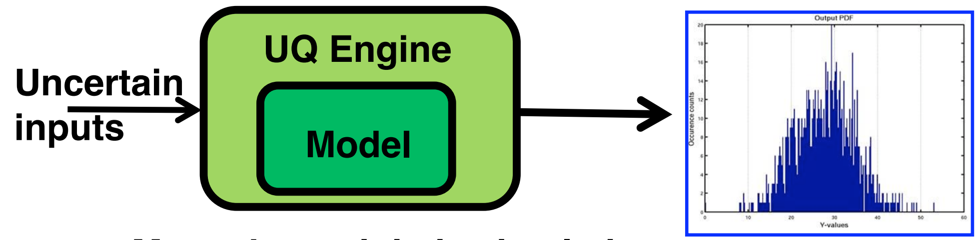
Different approaches to propagate uncertainties

- **Intrusive approach**



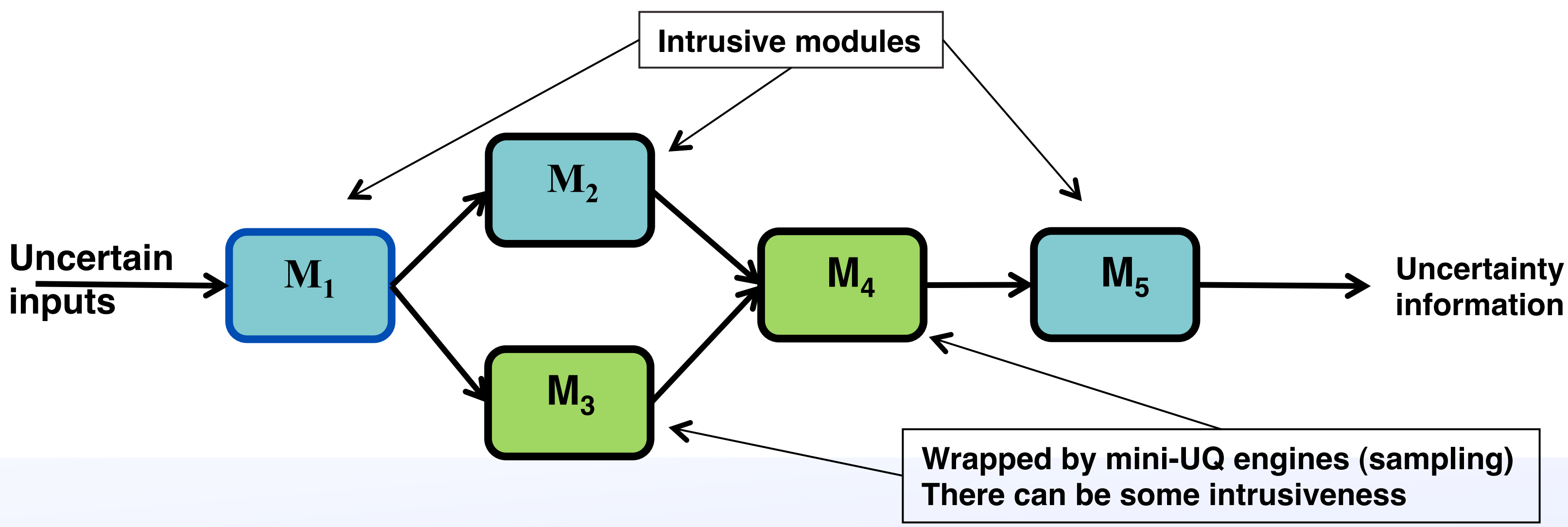
Stochastic simulation
(UQ embedded in the model)

- **Non-intrusive approach**



Many deterministic simulation

- **hybrid approach for multi-physics (one scenario)**



Propagation

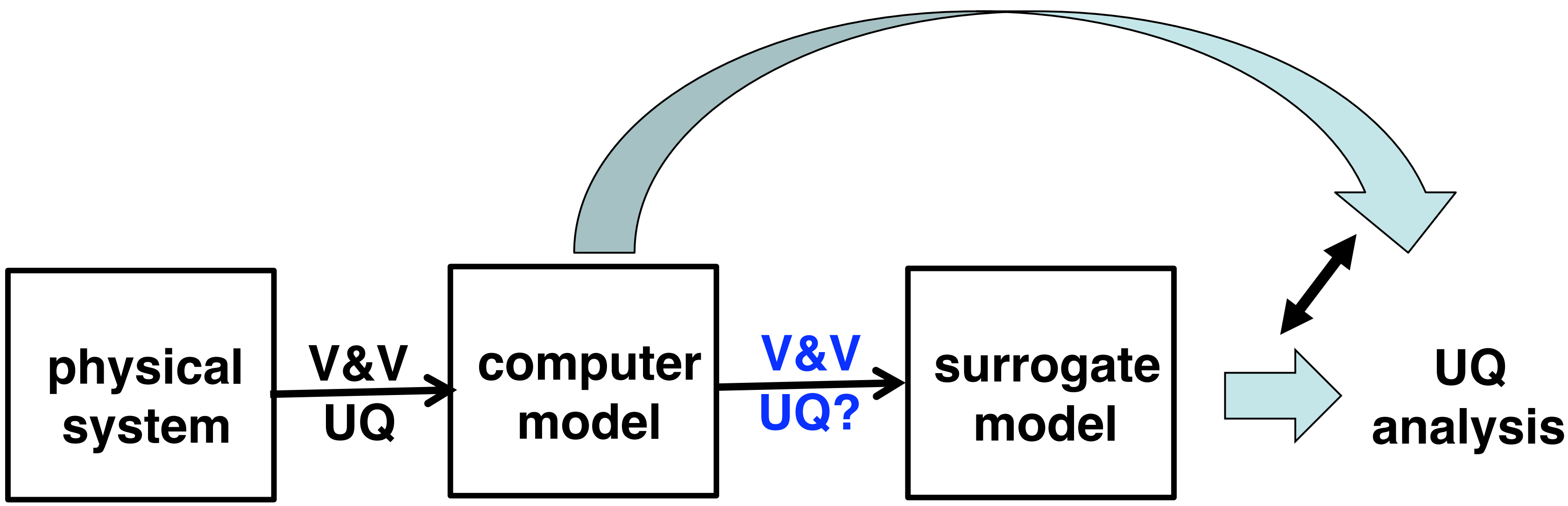
UQ development categories

- Forward propagation
- Data fusion/parameter estimation/calibration
- Input dimension reduction/variable subset selection
- Output dimension reduction
- Response surface analysis
- Sensitivity analysis (global/local, parameter/component)
- Risk analysis
- Data assimilation
- UQ software design

<u>UQ science is multi-disciplinary in nature</u>

- computational math
- applied statistics
- computer science (e.g. machine learning)
- domain science

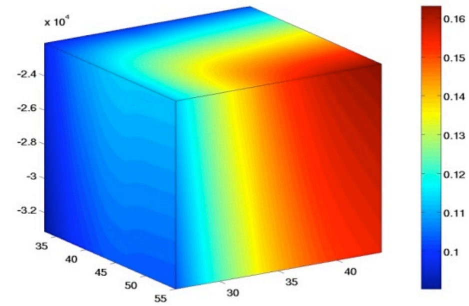
The role of surrogate models



- Once a good surrogate model is available, many tasks such as forward propagation and global sensitivity analysis can be computed cheaply.
- Q: How best should the surrogate model be validated and its uncertainties quantified?

Elements of a response surface method

- Sampling methods
  - Space-filling designs
  - Special points for specific functions
    (e.g. central composite, collocation points)



- Hypothesis function space (curve-fitting methods)
  - Polynomial regression, non-intrusive polynomial chaos
  - Splines (number of basis, degree of interaction)
  - Gaussian process (covariance function)
  - Artificial neural network, …..
- Response surface validation
  - Training error
  - Hold-out
  - Cross validations
  - Prediction errors (GP)
  - Goal-oriented metrics

Active research in

- computational math
  grad-based, sparse grids
- statistics (e.g. GP)
- machine learning

Challenges in response surface methods

- Come up with an accurate mapping
  - It is a model (surrogate) selection problem
  - Using as few sample points as possible
- Curse of dimensionality
  - Complexity grows exponentially as the no. of parameters
  - Boundary coverage
- Abrupt changes/discontinuities
  - In search of effective adaptive methods
- Combination of model form & parametric uncertainties
  - Combinatorial problem
- Practical questions:
  - how to handle failed sample points?
  - how to detect outliers?

Two Response Surface Approaches

- **Passive learning**

Generate a sample $X=\{X^i, i=1,\ldots N\ , X^i \in R^m\}$
Evaluate $S=\{(X^i, Y^i), i=1,\ldots N\ , X^i \in R^m, Y^i \in R\}$
Find $f \subset F$ **(hypothesis function space) such that** $V(S,f)$ **(some error measure) is minimized.**

- **Active Learning (adaptive)**

k = 0, $S=\Phi$
While tolerance not satisfied
Generate a sample $X_k=\{X_k^i, i=1,\ldots N_k\ , X_k^i \in R^m\}$ **given S**
Evaluate $S_k=\{(X_k^i, Y_k^i), i=1,\ldots N_k\ , X_k^i \in R^m, Y_k^i \in R\}$
$S=\{S, S_k\}$
Find $f_k \subset F$ **(hypothesis function space) such that** $V(S, f_k)$ **(some error measure) is minimized.**
check error measure for convergence, k = k + 1

Uniform And/or Adaptive refinements

General purpose methods??
(MARS with bootstrapping)

We can borrow some theory from machine learning (Castro, Willett and Nowak)

- **Define**
  - **m: number of parameters, n: sample size, sample point i:** X_i
  - **Sampling strategy (using n point):** S_n **, Function estimator:** f_n
- **Consider a function which is Holder smooth with Σ(L, α)**

$$\exists \varepsilon > 0 : \forall z \in [0,1]^m : \|z\text{-}x\| < \varepsilon \Rightarrow \|f(z)\text{-}P_k(z)\| \leq L\|z - x\|^{\alpha} ; k = (\underline{\alpha})$$

- **Main result from passive learning:**

$$\inf_{(f_n, S_n) \in passive} \sup_{f \in \Sigma(L,\alpha)} Error(\|f_n - f\|^2) \geq c n^{-2\alpha/(2\alpha+m)}$$

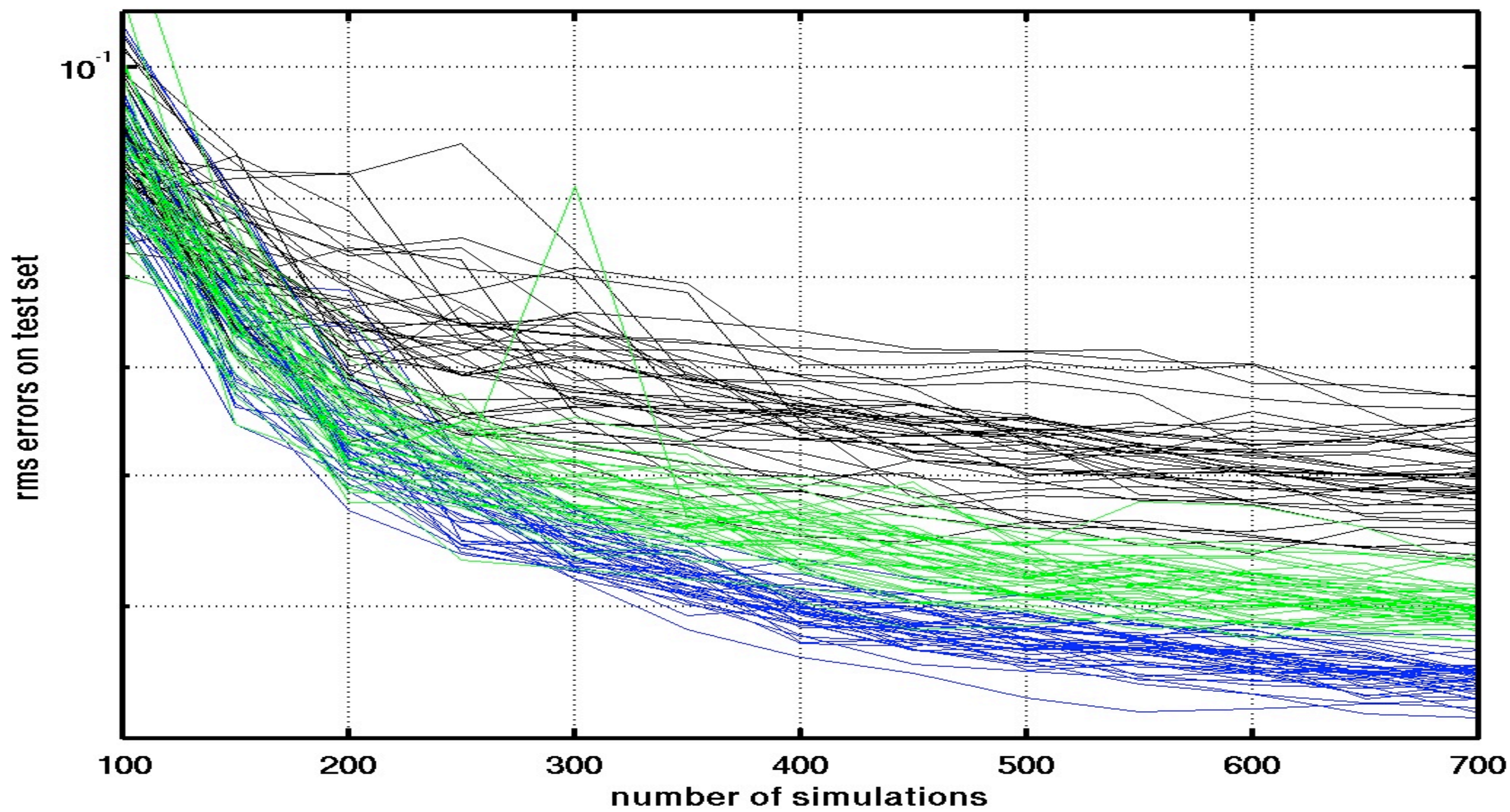
- **Active learning:**

$$X_i \sim P(X_i | X_1 \ldots X_{i-1}, Y_1 \ldots Y_{i-1})$$

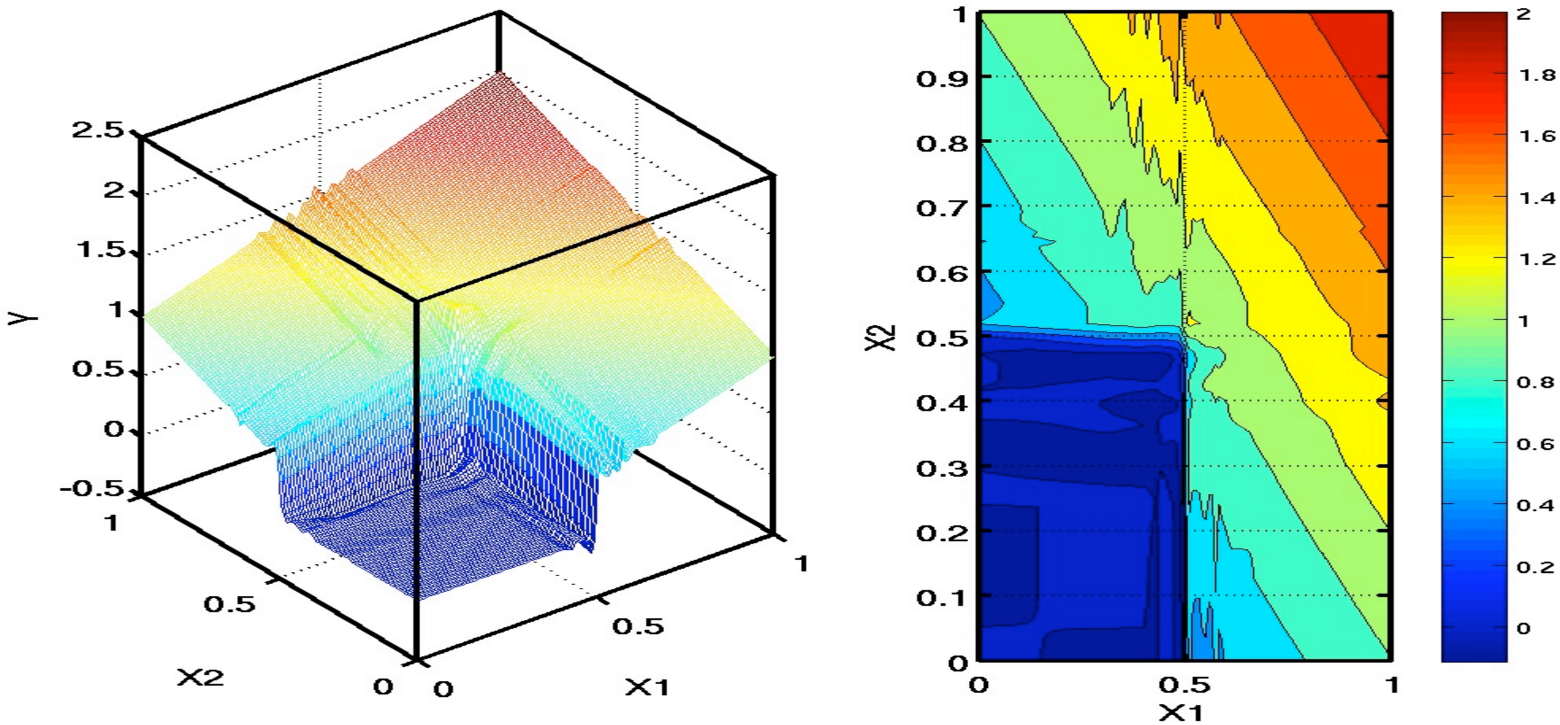
- **Active learning result:** $\inf_{(f_n, S_n) \in active} \sup_{f \in \Sigma(L,\alpha)} Error(\|f_n - f\|^2) \geq c n^{-2\alpha/(2\alpha+m)}$
- **Thus, when a function is spatially homogeneous, active learning has little advantage over passive learning. Active learning is appealing for piecewise constant/smooth functions.**

Convergence results for Test Problem 3

mars w/ bag. Green: mars w/ NN variance black: random pick



Test Problem 3: An 2-parameter function with discontinuity



$$Y = \begin{cases} 0 & X_1 < 0.5, X_2 < 0.5 \\ X_1 + X_2 & otherwise \end{cases}$$

- 100 to 700 points at an increment of 50
- each method is run 40 times (random initial sample)
- use a validation data set of 5000 points

Dimension reduction methods are used to compress or down-select the large number of uncertain parameters

- **Spatial-temporal randomness**
  - e.g. random variable B(x) defined on the spatial domain
  - usually comes with spatial correlation (covariance function)
  - reduce dimension via principal component analysis (KL)
- **Reduce the dimension of the output variables**
  - methods based on PCA and kernel PCA
- **Reduce the number of physics parameters**
  - the goal is to select a subset of "sensitive" parameters (features)
  - also called variable subset selection (VSS)
  - methods from computational math, statistics, machine learning
  - parametric and nonparametric methods

Variable subset selection methods

Let $X \in R^m$, design and evaluate $S=\{(X^i, Y^i), i=1,\ldots N\}$.
Select $X_G \subset X$ such that $I(X,Y) \cong I(X_G, Y)$ where $I(X,Y)$ is the information that X_G brings about Y .

Assumptions/ objectives

- **Methods based on linearity assumptions**
  - Standardized regression coefficient or SRC
  - Plackett-Burman
  - derivative-based local sensitivity analysis
- **Methods based on monotonicity assumptions**
  - Spearman rank correlation coefficient
- **Non-parametric ethods based on global smoothness assumptions**
  - surrogate-based methods (spline or kriging)
  - Morris method
  - tree-based methods (BART, CART)
- **Non-parametric methods based on local smoothness assumptions**
  - Delta test (based on nearest neighbors)
  - tree-based methods
- **Other methods: data rich methods (under-determined: regularization)**

An Example Comparing Different VSS Methods

Method	Size = 55	Size = 110	Size = 220	
SPEA	14	9	13	
Morris	94	100	100	✓
MARS	97	100	100	✓
MARS+VD	98	100	100	✓
Delta Test	100	100	100	✓
SumOfTrees	72	96	100	✓

Data: number of successes out of 100 runs
SPEA does not work well probably due to non-monotonicity

$$Y = 10\sin(\alpha X_1 X_2) + 20(X_3 - 0.5)^2 + 10X_4 + 5X_5 + \varepsilon, X \in [0,1]^{10}, \alpha = 2$$

Another Example Comparing Different VSS Methods

Method	Size = 210	Size = 420
SPEA	0	0
Morris	6	24
MARS	3	22
MARS+VD	3	18
Delta Test	17	61
SumOfTrees	1	3

✓

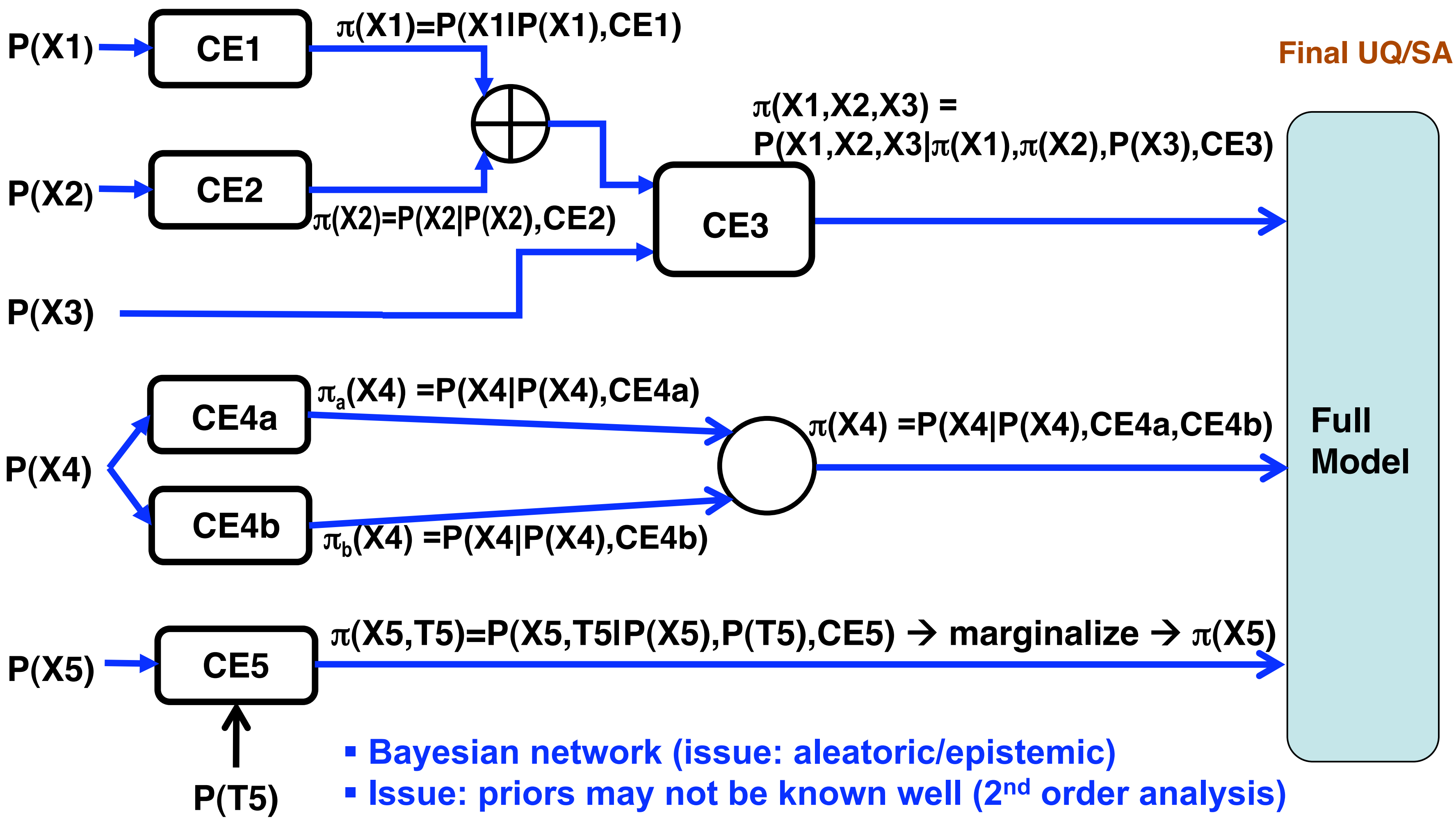
Problem characteristics: active region 1/32 of domain
Noise dominates and pollutes all methods

$$Y = \begin{cases} \sum_{i=1}^{5} \sin(2\pi X_i) + \varepsilon, if \quad X_i < 0.5, i = 1,..,5 \\ \varepsilon, \qquad otherwise \end{cases}$$

Need a unified framework for data fusion at different stages/ levels

- Component physics level (plenty)
  - turbulence models
  - material models (some physics-based, some empirical)
  - Some of these are from focused experiments (e.g. a different experimental setup but with the same materials) which in turn have their own uncertainties outside the model in consideration
- Subsystem level (some)
  - e.g. Multiple material models + fluid dynamics
- Full system level (scarce)
  - Some of which may be unreliable (large errors)
  - These data may become less relevant with time

A framework for multi-stage data fusion/calibration



Prior input Distributions (independent)

- Bayesian network (issue: aleatoric/epistemic)
- Issue: priors may not be known well (2^{nd} order analysis)
- Software design (flexible, compatible, data movement)
- systematic errors

CE: focused experiments

The building blocks of a global sensitivity analysis methodology

- **Methods and sampling strategies (arbitrary posteriors)**
  - **first order** $V = V[E(Y \mid X_i)] + E[V(Y \mid X_i)]$
    - **replicated Latin hypercube (or random)**
    - **response surface + direct numerical integration**
  - **second order** $V = V[E(Y \mid X_i, X_j)] + E[V(Y \mid X_i, X_j)]$
    - **replicated orthogonal array (or random)**
    - **response surface + direct numerical integration**
  - **total order** $V = V[E(Y \mid X_{-i})] + E[V(Y \mid X_{-i})]$
    - **extended Fourier Amplitude Sampling Test**
    - **response surface + direct numerical integration**
  - **group** $V = V[E(Y \mid \{X_i\})] + E[V(Y \mid \{X_i\})]$
    - **response surface + direct numerical integration**

$$\eta^2_{X_i} = \int \left[\int F(X_{\sim i}|X_i)\, p(X_{\sim i}|X_i)\, dX_{\sim i} - \mu(F) \right]^2 p(X_i)\, dX_i$$

Software design issues in putting all these together

Confidence interval analysis
Orthogonal arrays
Cross validation
Principal component analysis
Correlation analysis
Latin hypercube
Screening designs
Space-filling designs
Gaussian process
Graphical analysis
Nonparametric testing
Kolmogorov Smirnov test
Derivative-based methods
Constrained optimization
Probability distributions
Support vector machines
Delta test
Factorial design
Second order sensitivity indices
Sobol' decomposition
Manifold mapping optimization
Multivariate splines

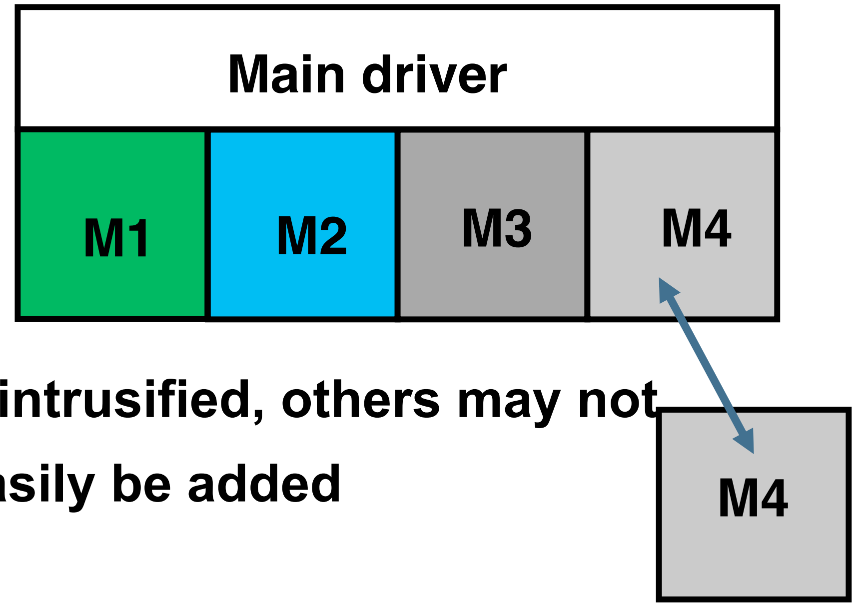
Main effects
Adaptive response surfaces
Sparse grids
Total sensitivity indices
Markov chain Monte Carlo
Reliability analysis
Fourier amplitude sampling test
Artificial neural networks
Bayesian Sensitivity analysis
Regression analysis
Analysis of variance

A Problem Solving Environment for Uncertainty Analysis and Design Exploration

Many other challenges

- Validation metrics
- Quantifying extrapolation uncertainties
- Validation of UQ methods (self-validation?)
- Model form uncertainties
- Guidelines for formulating UQ approach
- How to study uncertainties and errors together
- Many challenges in the intrusive and hybrid worlds
- …….

Challenges and Opportunities for Hybrid UQ



- Flexibility
  - support “plug-and-play”
  - support progressive code enhancement
  - some sub-models may easily be intrusified, others may not
  - new uncertain parameters can easily be added
- Mathematical rigor
  - intrusifying sub-models increases mathematical understanding
  - facilitate uncertainty tracking between sub-models
- Less challenges compared to fully intrusive methods?
  - difficult parts of the model can use non-intrusive methods
  - model developers need not understand UQ for the whole system
  - easier to debug codes

Research and Development Issues for hybrid UQ

- **Mathematics R&D**
  - **Uncertainty representation between modules**
  - **Error analysis of transformation between representations**
  - **Dimension reduction (uncertain parameters)**
  - **Sensitivity analysis (variance-based)**
  - **Calibration/data fusion (data available at module level)**
  - **different probability distributions for different variables**
  - **parallel linear solvers for intrusive modules**
- **CS R&D**
  - **tracking uncertainties throughout the simulation**
  - **application programming interface (wrapper) design**
  - **integration of non-intrusive UQ methods**
  - **scheduling/load balancing**
  - **fault tolerance**

THE END

Deadly Sins in UQ practice

1. Not exercising due diligence in understanding the limitations of the proposed UQ approaches
2. Not exercising due diligence in identifying key sources of uncertainties
3. Not exercising due diligence in characterizing the sources of uncertainties
4. Selecting UQ methods that do not match model characteristics
5. Sensitivity analysis has nothing to do with uncertainty quantification (you are just doing SA, and not UQ).
6. We can do UQ without using data.
7. Thinking that UQ is just math/statistics.

A few observations about multi-physics code development

- Usually begin with simple physics
  - Low fidelity, approximate physics & couplings
  - Many empirical sub-models
  - focus on mimicking key phenomena qualitatively
  - Strive for low computational cost
  - Operator splitting for ease of plug-and-play
- Progressive code enhancement: better physics
  - Better physics understanding
  - Validation shows inadequate fidelity
  - Advances in algorithms
  - Advances in hardware
- Many hidden assumptions
  - how to do a good job in identifying uncertainties

Fundamental formulas for UQ

$$p(Y)=\int p(Y|X)\,p(X)dX=\int \delta(Y-F(X))\,p(X)\,dX$$

$$\eta^2_{X_i}=\int\left[\int F(X_{\sim i}|X_i)p(X_{\sim i}|X_i)dX_{\sim i}-\mu(F)\right]^2 p(X_i)dX_i$$

$$\pi(X|D)\propto P(D|X)P(X)$$

$$\pi(X|D)=\int \pi(X,T|D)\,dT$$